

## REMARKS

Claims 37-72 are pending and stand rejected. Applicants have herein amended claims 37-72. Support for the amendments can be found throughout the specification of the present application, as well as its parent application (U.S. Ser. No. 09/595,650) and the provisional application to which it ultimately claims priority (U.S. Ser. No. 60/139,845), as described further below. No new matter has been added.

Applicants thank the Examiner for the courtesy of the helpful telephonic interview held on March 18, 2009. While no ultimate agreement on the claims was reached, the Examiner indicated orally on March 20 that his Interview Summary, while not yet available on PAIR, indicated that progress towards agreement was made.

Given the amendments above and the remarks herein, Applicants respectfully request reconsideration and allowance of the pending claims.

### Priority Rejections, New Matter Objections (Specification Objection), and Rejections under 35 U.S.C. § 112, first paragraph

The Examiner rejected previously pending claims 37-72 as lacking priority to the parent and provisional application; as introducing new matter; and as lacking written description. Applicants respectfully assert that the priority, new matter, and written description rejections can be addressed simultaneously herein. As amended, claims 37 and 55 recite a "computer running a computer program" or a "computer program in tangible form," respectively. The dependent claims have been modified to recite the appropriate terms. Support for the terms, both explicit and implicit, can be found in the publication of the present application (US 2004/0148149) at, for example, paragraphs [0014], [0020], [0026], [0027], [0030], [0031], [0043], [0044], [0046], [0050], [0055], [0056], Examples 1 and 2, Figures 1-7, the Tables, and the references incorporated by reference (*e.g.*, Pang *et al.*, JACS 121:1717-1725 (1999) and Stote and Karplus, Proteins 23:12-31 (1995) (also cited by the Examiner)). As the present specification is a divisional of its parent U.S. Ser. No. 09/595,650, the same support is also available in the parent case. Provisional Ser. No. 60/139,845 similarly supports the amendments and establishes

priority to June 18, 1999; *see, e.g.*, page 4, lines 10-14; page 5, lines 1-7 and lines 27-31; page 6, lines 10-22; page 10 (Example 1), lines 5-17 and Table 1; page 11, lines 1-9 and lines 21-25; page 12, lines 28-3; and the Tables and Figures. From this support, it would have been evident to a person having ordinary skill in the art, as of the priority date of June 18, 1999, that the inventors used a computer running a computer program, *e.g.*, a modified AMBER™ 5.0 program, to generate the molecular modelling simulation results as described in the present specification (*see* Examples 1 and 2 and Figures 1-7), and thus that the inventors had support for and possession of the claimed subject matter as amended.

Accordingly, Applicants respectfully request withdrawal of the priority rejections, new matter objections, and written description rejections.

#### Rejections under 35 U.S.C. § 101

The Examiner rejected claims 37-72 as directed to non-statutory subject matter, as the term "data storage medium" could allegedly encompass carrier waves. Applicants respectfully assert that the amended claims do not encompass intangible media, and request withdrawal of the rejections.

#### Rejections under 35 U.S.C. § 103(a)

The Examiner rejected claims 37-47, 52-65, and 70-72 as obvious over Andriotis *et al.*, Chemical Physics Letters 301:503-508 (1999) ("Andriotis") in view of Stote *et al.*, Proteins 23:12-31 (1995) ("Stote"), with claims 48-51 and 66-69 as obvious when Andriotis in view of Stote are taken in further view of Aqvist *et al.*, Journal of the American Chemical Society 112:2860-2868 (1990) ("Aqvist"). In particular, the Examiner alleged that Andriotis simulated nickel-carbide clusters, where the central atom was carbon having a radius greater than zero and the dummy atoms were nickel, which were positively charged and had a radius of about zero, and Stote demonstrated zinc binding studies with the use of various computer workstations. Accordingly, the Examiner alleged it would have been obvious to a person having ordinary skill

in the art at the time of the present invention to modify the nickel-carbide clusters of Andriotis by use of advanced computer systems of Stote, with a reasonable expectation of success.

Applicants respectfully disagree. As amended claims 37 and 55 recite that a monoatomic metal ion is simulated as “a metal molecule”, where the “metal molecule comprises a plurality of atoms comprising a center atom and one or more dummy atoms, where the center atom has a van der Waals radius greater than zero and has a charge of zero, where the center atom is covalently linked to said one or more dummy atoms, and where each dummy atom has a positive charge.” Andriotis does not teach or suggest such a metal molecule simulation of a monoatomic metal ion, particularly where the center atom has a charge of zero. The metal carbide clusters of Andriotis include non-metallic atoms (the carbons), and thus do not represent simulations of a monoatomic metal ion as a metal molecule, as required by the present claims. Moreover, Andriotis' clusters have center atoms (carbons) that do not have a “charge of zero.” Neither Stote nor Aqvist cure the deficiencies of Andriotis in this regard, as neither provides any rationale to modify the clusters of Andriotis so that a monoatomic metal ion of Andriotis is simulated as a metal molecule, let alone as a metal molecule where a center atom of the metal molecule has a charge of zero.

Given all of the above, Applicants respectfully request withdrawal of the rejections under 35 U.S.C. § 103(a).

### CONCLUSION

Applicants respectfully assert that the present claims are in condition for allowance, which action is hereby requested. The Examiner is invited to telephone the undersigned attorney if such would expedite prosecution.

Included herewith are a Petition for Extension of Time (Two Months) and Fee. No other fee is believed due. Please charge Deposit Account No. 06-1050 for any other charges or credits.

Respectfully submitted,

Date: \_\_\_\_\_

3/23/2008



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